Supplementary data for article:

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Mutual influence of parallel, CH/O, OH/π and lone pair/π interactions in water/benzene/water system

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Supplementary information

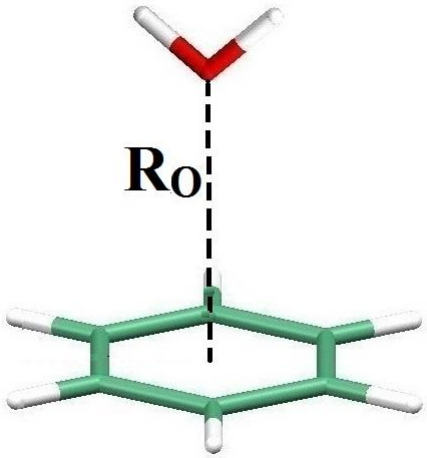

Fig. S1. Water/benzene dimer with established lone pair/π interaction; R_O is the distance between water oxygen atom and benzene ring centroid; the geometry shown has R_O distance of 3.4 Å

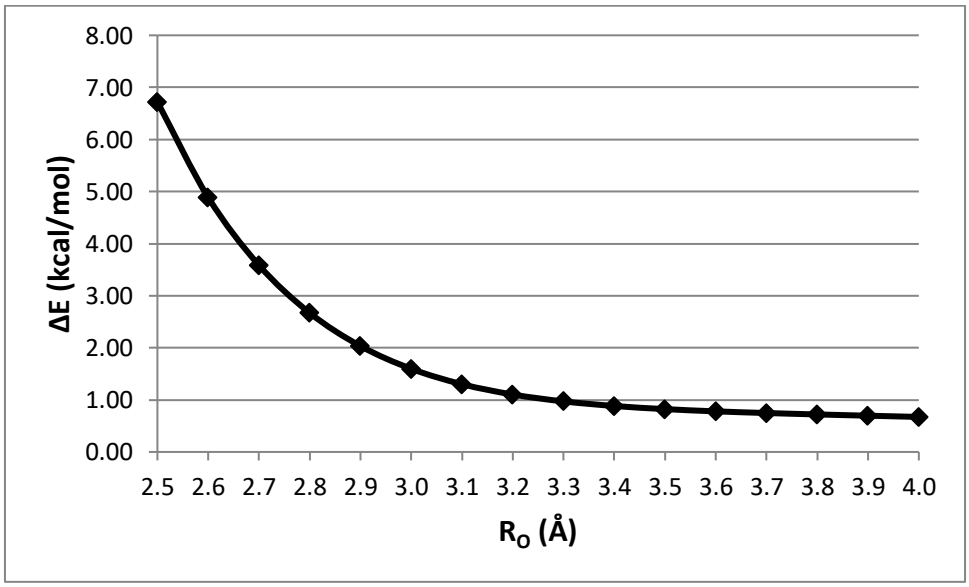

Fig. S2. Water oxygen···benzene centroid distance (R_O) dependence of interaction energy of water/benzene lone pair/π interaction (Fig. S1), calculated at MP2/cc-TZVP level with BSSE correction